**NATIONAL UNIVERSITY OF SINGAPORE**

# PC3236 – COMPUTATIONAL METHODS IN PHYSICS

(Semester II: AY 2015-16)

Time Allowed: 2 Hours

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**<u>INSTRUCTIONS TO CANDIDATES</u>**

1. Please write your student number only. **Do not write your name.**
2. This examination paper contains FOUR questions and comprises FOUR printed pages.
3. Answer ALL questions.
4. All questions carry equal marks.
5. Answers to the questions are to be written in the answer books.
6. Show all working steps clearly.
7. Please start each question on a new page.
8. This is a CLOSED BOOK examination.
9. Programmable or graphic calculators are **NOT** allowed to be used in this examination.
10. The last page contains a list of formulae.

1. (a) Evaluate the following integral by Romberg integration

$$\int_0^1 \frac{e^{-x}}{\sqrt{1-x}}\,dx.$$

Express your answer accurate to at least three decimal places.

(b) Given the following data, $f(0.3)$ is approximated by polynomial interpolation.

| $x$ | 0.0 | 0.2 | 0.4 | 0.6 |
|---|---|---|---|---|
| $f(x)$ | 15.0 | 21.0 | 30.0 | 51.0 |

Suppose it is discovered that $f(0.4)$ was understated by 10 and $f(0.6)$ was overstated by 5. By what amount should the approximation to $f(0.3)$ be changed?

2. (a) Use the secant method to determine the root of

$$2x\cos(2x) - (x-2)^2 = 0,$$

that lies in the interval $(2, 3)$. Express your answer accurate to at least four decimal places.

(b) Evaluate the integral

$$\int_0^1 \int_0^1 \frac{x\cos(y)}{x+y}\,dx\,dy,$$

using the two-point Gauss-Legendre rule.

(c) Find the Padé approximation $R_{2,2}(x)$ for $f(x) = \ln(1+x)/x$. You may use the Maclaurin expansion

$$f(x) = 1 - \frac{x}{2} + \frac{x^2}{3} - \frac{x^3}{4} + \frac{x^4}{5} - \cdots$$

3. Using a finite difference method, solve the wave equation

$$\frac{\partial^2 u}{\partial t^2} = 16\frac{\partial^2 u}{\partial x^2}, \quad 0 \le x \le 1,$$

subject to the following conditions

$$u(x,0) = \sin(\pi x/4), \qquad \frac{\partial u}{\partial t}(x,0) = 0,$$

$$u(0,t) = 0, \qquad \frac{\partial u}{\partial x}(1,t) = \frac{\pi}{4\sqrt{2}}\cos(\pi t),$$

Use a spatial step size $h = 0.2$ and a temporal step size $\tau = 0.05$. Compute for three time steps.

4. Solve the following boundary value problem

$$\frac{d^2 y}{dx^2} + y^2 = 6x, \quad y(0) = 0, \quad y(1) = 1,$$

with the finite difference method. Discretize the spatial domain using a step size of 0.2. Ensure that your answers have converged to at least 3 decimal places.

LHS

## Formulae Sheet

Taylor series:

$$f(x) = f(a)+(x-a)f'(a)+\frac{(x-a)^2}{2!}f''(a)+\cdots+\frac{(x-a)^{n-1}}{(n-1)!}f^{[n-1]}(a)+\frac{(x-a)^n}{n!}f^{[n]}(\xi)$$

Inverse quadratic interpolation:

$$x(f) = \frac{(f-f_2)(f-f_3)}{(f_1-f_2)(f_1-f_3)}x_1 + \frac{(f-f_1)(f-f_3)}{(f_2-f_1)(f_2-f_3)}x_2 + \frac{(f-f_1)(f-f_2)}{(f_3-f_1)(f_3-f_2)}x_3$$

Secant method: $x_{i+1} = x_i - f(x_i)\dfrac{x_i - x_{i-1}}{f(x_i)-f(x_{i-1})}$

Newton's method for system of equations: $\boldsymbol{J}(\boldsymbol{x})\boldsymbol{\Delta x} = -\boldsymbol{f}(\boldsymbol{x})$, $\boldsymbol{J}$ is the Jacobian matrix

Central difference: $f'(x) = \dfrac{f(x+h)-f(x-h)}{2h}$, $f''(x) = \dfrac{f(x+h)-2f(x)+f(x-h)}{h^2}$

Richardson extrapolation: $F = \dfrac{(h_1/h_2)^p D(h_2) - D(h_1)}{(h_1/h_2)^p - 1}$

Padé: $R_{n,m}(x) = \dfrac{\sum_{i=0}^{n} p_i x^i}{1+\sum_{j=1}^{m} q_j x^j}$, $\displaystyle\sum_{i=0}^{k} a_i q_{k-i} = p_k$, $k = 0, 1, \ldots, N$ and $N = n+m$

Lagrange: $p(x) = \displaystyle\sum_{j=1}^{n} l_{j,n}(x) f(x_j)$, $l_{j,n}(x) = \dfrac{(x-x_1)(x-x_2)\cdots(x-x_{j-1})(x-x_{j+1})\cdots(x-x_n)}{(x_j-x_1)(x_j-x_2)\cdots(x_j-x_{j-1})(x_j-x_{j+1})\cdots(x_j-x_n)}$

Simpson's 1/3 rule: $\displaystyle\int_a^b f(x)\,\mathrm{d}x = \left[f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right]\frac{h}{3}$

Monte Carlo: $\displaystyle\int_a^b f(x)\,\mathrm{d}x \approx (b-a)(\langle f\rangle_N \pm \sigma_N)$, $\sigma_N = \sqrt{\dfrac{\frac{1}{N}\sum_i f(x_i)^2 - \left(\frac{1}{N}\sum_i f(x_i)\right)^2}{N-1}}$

Modified Euler: $y(x_0+h) = y(x_0) + hf(x_{\mathrm{mid}}, y_{\mathrm{mid}})$

Heun's method: $y(x_0+h) = y(x_0) + h\dfrac{f_0 + f(x_0+h, y_0+hf_0)}{2}$

Crank-Nicolson method: $y(x_0+h) = y(x_0) + \dfrac{h}{2}(f_0+f_1)$

Leibniz Integral Rule: $\dfrac{\mathrm{d}}{\mathrm{d}x}\displaystyle\int_{a(x)}^{b(x)} f(x,y)\,\mathrm{d}y = \int_{a(x)}^{b(x)} \frac{\partial f}{\partial x}\,\mathrm{d}y + f(x,b(x))\frac{\mathrm{d}b}{\mathrm{d}x} - f(x,a(x))\frac{\mathrm{d}a}{\mathrm{d}x}$

Gauss-Legendre quadrature:

$$\int_{-1}^{1} f(\xi)\,\mathrm{d}\xi \approx \sum_{i=1}^{n} W_i f(\xi_i),$$

| $\pm\xi_i$ | $W_i$ | $\pm\xi_i$ | $W_i$ |
|---|---|---|---|
| $n=2$ | | $n=3$ | |
| $\frac{1}{\sqrt{3}}$ | 1 | 0 | $\frac{8}{9}$ |
| | | $\sqrt{\frac{3}{5}}$ | $\frac{5}{9}$ |

– END OF PAPER –